Microscopic Approaches to Level Densities

Erich Ormand
Nuclear Theory and Modeling
Livermore

Calvin Johnson
San Diego State University

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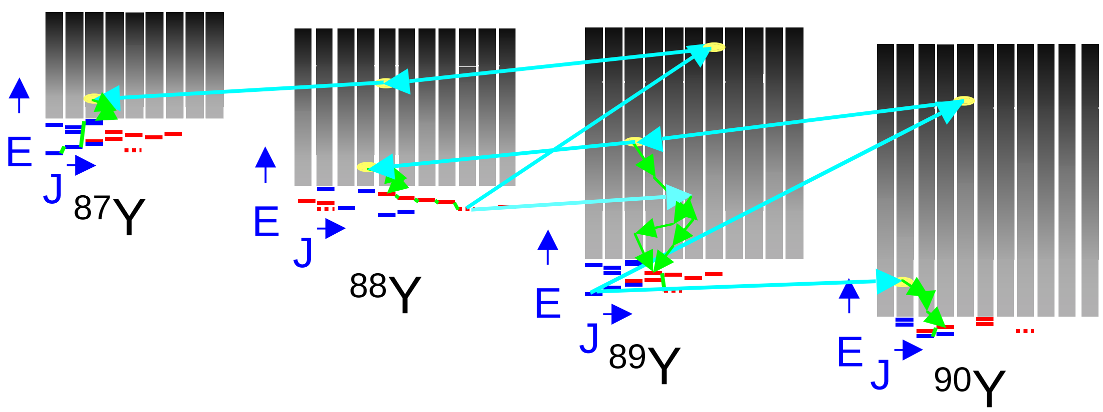
Level Densities

- **Number of levels per MeV of excitation**
  - **Formally**

$$\rho(E) = tr\left[\delta\left(E - \hat{H}\right)\right] = \sum_i \langle \psi_i | \delta\left(E - \hat{H}\right) | \psi_i \rangle$$

$$= -\frac{1}{\pi} \mathrm{Im}\, tr\left[\frac{1}{E - \hat{H} + i\eta}\right]_{\eta \to 0}$$

  - **State density (includes *2J+1* degeneracy)**
- **Phase-space determines the rate of reactions and decays**
  - **Compound reactions: (n,g), (n,n'), (n,2n) …, Nucleosynthesis**



Reaction cross sections

- **Hauser-Feshbach**
  - **— Channel c to c’**

$$\frac{d\sigma_{cc'}}{dE_{c'}} = \sum_{J,\Pi} \sigma_c^{comp} \frac{\sum_{l'} g_{l'J_{c'}} T_{l'}\left(E_{c'}\right)\rho\left(E_{c'}^{\max} - E_{c'}\right)}{\sum_{c''l''} g_{l''J_{c''}} T_{l''}\left(E_{c''}\right) \int_{o}^{E_{c'}^{\max}} \rho\left(E_{c''}^{\max} - E_{c''}\right) dE_{c''}}$$

$$\sigma_c^{comp} = \frac{\pi}{k_c^2} g_J \left\{ \sum_{s,l} T_l(c) \right\} - \sigma_c^{preeq}$$

- **Physics inputs**
  - **— Discrete states**
  - **— Level density**
  - **— γ-ray decay path; low-lying discrete spectroscopy, isomers**
    - **– Transition from continuous to discrete spectrum**
  - **— Transmission coefficients - optical model - far from stability**
  - **— Pre-equilibrium cross section - angular momentum deposition**
  - **— Fission**

A fast and accurate model for $\rho(E)$ is needed
Especially for nuclei far from stability

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Level Densities

- **Usual approach:**
  - **Gilbert and Cameron**
    - **Small set of discrete states up to E_{cut}**
    - **Finite temperature below E_{match}**
    - **Fermi gas above E_{match}**
  - **Fix parameters with some known data**
    - **Difficult to extrapolate to nuclei with no data – uncontrolled far from stability**
- **Microscopic treatment of H_{res}**
  - **Count single-particle states in the deformed mean-field**
    - **Need *ad hoc* collective enhancement factors**
  - **Shell Model**
    - **Direct diagonalization**
      - **Too many states!**
    - **Monte Carlo Shell Model**
      - **Sign problem**
        - **Schematic interactions: SDI or pairing plus quadrupole**
    - **Statistical methods**
      - **Moments of H_{res} with some assumptions on the form of the level density**

Level Densities: the nuclear shell model

- **Goal is to accurately describe low-lying structure**
  - — **Eigenvalues of Hamiltonian matrix** $H_{ij}=\langle\psi_i|H|\psi_j\rangle$

$$\begin{pmatrix} H_{\alpha\alpha} & H_{\alpha\beta} & H_{\alpha\gamma} & H_{\alpha\delta} \\ H_{\beta\alpha} & H_{\beta\beta} & H_{\beta\gamma} & H_{\beta\delta} \\ H_{\gamma\alpha} & H_{\gamma\beta} & H_{\gamma\gamma} & H_{\gamma\delta} \\ H_{\delta\alpha} & H_{\delta\beta} & H_{\delta\gamma} & H_{\delta\delta} \end{pmatrix}$$

- **Ensemble averages**

$$h_\alpha = \frac{1}{N_\alpha}\sum_i H_{i\alpha,i\alpha}$$

$$\Gamma_{\alpha\beta} = \frac{1}{N_\alpha\left(N_\beta + \delta_{\alpha\beta}\right)}\sum_{ij} H_{i\alpha,j\beta}H_{j\beta,i\alpha} - h_\alpha^2\delta_{\alpha\beta}$$

- **Lanczos**

$$\begin{aligned} \hat{H}\mathbf{v}_1 &= \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2 \\ \hat{H}\mathbf{v}_2 &= \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3 \\ \hat{H}\mathbf{v}_3 &= \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4 \\ \hat{H}\mathbf{v}_4 &= \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5 \end{aligned}$$

$$\left\langle \mathbf{v}_1 \right| \frac{1}{E-\hat{H}} \left| \mathbf{v}_1 \right\rangle = \cfrac{1}{E-\alpha_1-\cfrac{\beta_1^2}{E-\alpha_2-\cfrac{\beta_2^2}{E-\alpha_3-\cfrac{\beta_3^2}{0}}}}$$

Monte Carlo Shell Model

- **Start with thermodynamics**

$$E(\beta) = \frac{\mathrm{Tr}\left(\hat{H}e^{-\beta\hat{H}}\right)}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right)} = \frac{\int dEE\rho(E)e^{-\beta E}}{\int dE\rho(E)e^{-\beta E}}$$

$$\ln Z(\beta) = -\int_0^\beta d\beta' E(\beta') + \ln Z(0)$$

$$\rho(E) = \frac{1}{2\pi}\int_{-i\infty}^{i\infty} Z(\beta)e^{\beta E}d\beta \quad \approx \quad \frac{e^{-\beta_0 E + \ln Z(\beta)}}{2\pi\sqrt{\left|\partial^2 Z/\partial\beta^2\right|_{\beta=\beta_0}}}, \qquad E = -\frac{\partial \ln Z(\beta)}{\partial\beta}$$

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Monte Carlo Shell Model

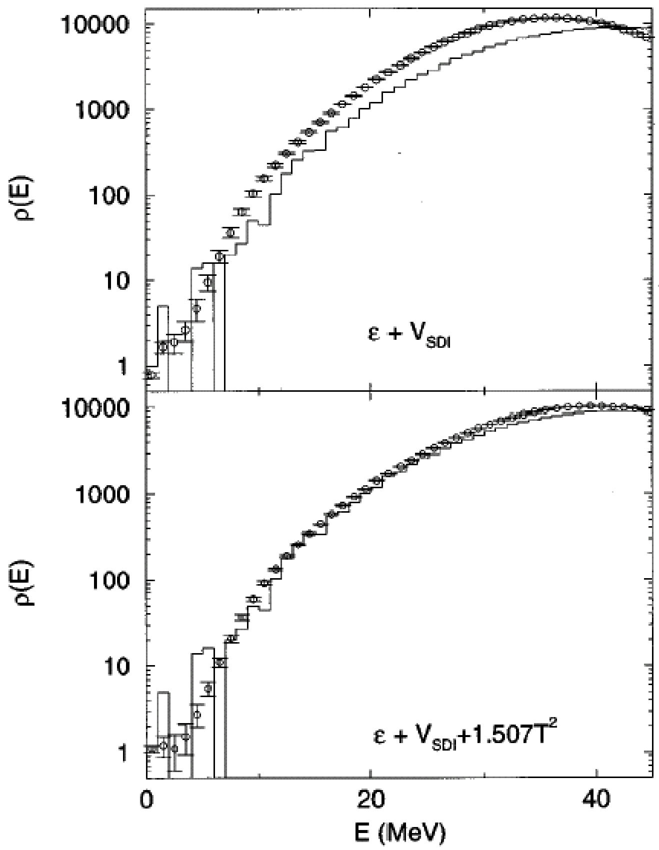
- **Can't handle the two-body part:** $e^{-\beta\hat{H}} = e^{-\beta\sum_{\nu} V_\nu \hat{O}_\nu^2}$
- **Use Gaussian integral:** $e^{\frac{1}{2}\Lambda\hat{O}^2} = \sqrt{\frac{|\Lambda|}{2\pi}}\int d\sigma e^{-\frac{1}{2}|\Lambda|\sigma^2 + \sigma\Lambda\hat{O}}$
- **Then** $e^{-\beta\hat{H}} = \int D[\sigma] e^{-\frac{1}{2}\beta\sum_{\nu}|V_\nu|\sigma_\nu^2} e^{-\beta\hat{h}(\sigma)}$

$$\langle\hat{O}\rangle(\beta) = \frac{\int D[\sigma] e^{-\frac{1}{2}\beta\sum_{\nu}|V_\nu|\sigma_\nu^2}\,\mathrm{Tr}\left[e^{-\beta\hat{h}(\sigma)}\right]\mathrm{Tr}\left[e^{-\beta\hat{h}(\sigma)}\hat{O}\right]\Big/\mathrm{Tr}\left[e^{-\beta\hat{h}(\sigma)}\right]}{\int D[\sigma] e^{-\frac{1}{2}\beta\sum_{\nu}|V_\nu|\sigma_\nu^2}\,\mathrm{Tr}\left[e^{-\beta\hat{h}(\sigma)}\right]}$$

- **Solve using Monte Carlo sampling**
  - — **Accurately evaluates *ρ(E)***
  - — **Problems:**
    - – **Sign is bad for arbitrary interactions**
    - – **Slow**

Application of the Monte Carlo Shell Model

- **W.E. Ormand, PRC56, R1682 (1997) – ^{24}Mg**



- **H. Nakada and Y. Alhassid, PRL79, 2939 (1997)**

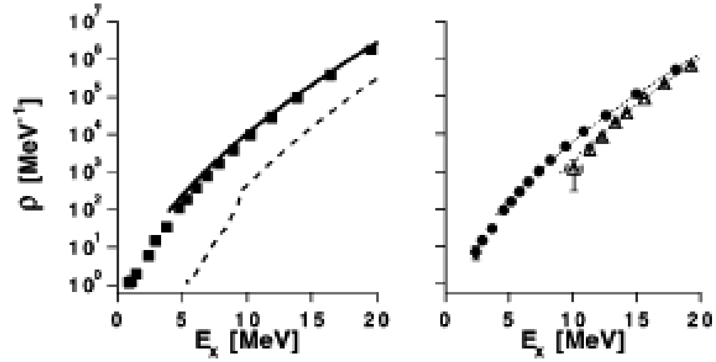


FIG. 3. Level densities of ^{56}Fe. Left: total level density. The SMMC level density (solid squares) is compared with the HFA level density (dashed line). The solid line is the experimental level density [20]. Right: positive- and negative-parity level densities in the SMMC. The conventions are as in Fig. 1 inset. The dotted lines are the fit to Eq. (1) with the parameters quoted in the text.

Statistical Method #1: Pluhar & Weidenmüller - 1

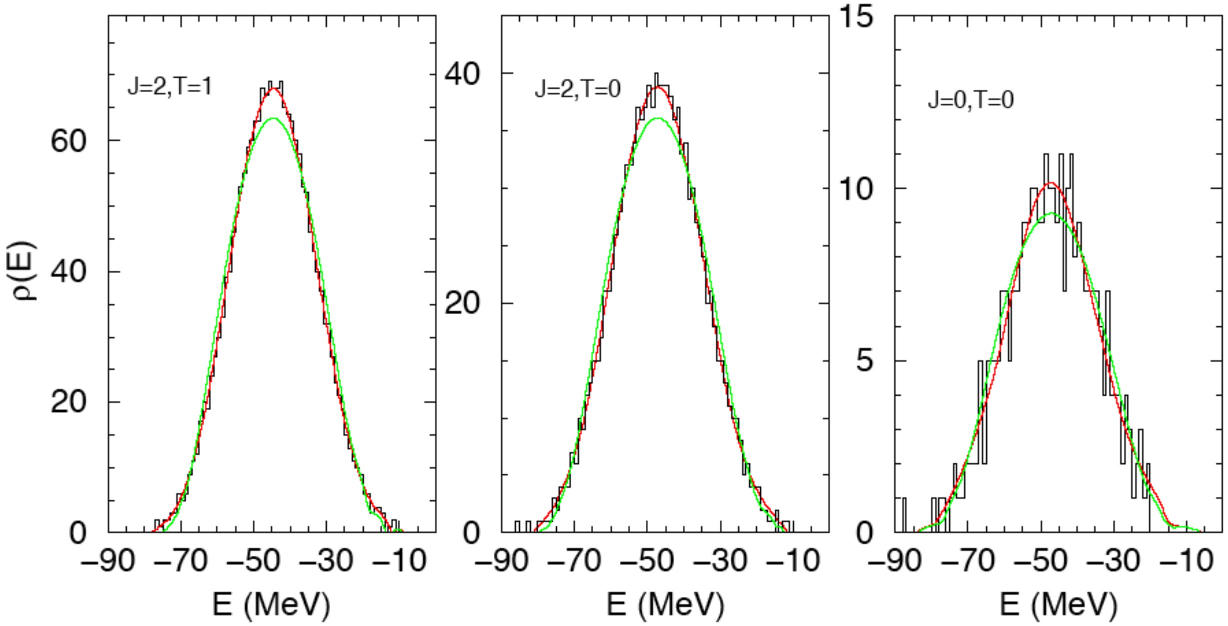
- **Shell Model**
  - — **Construct basis states ψ_i**
  - — **Diagonalize Hamiltonian matrix $H_{ij}=\langle\psi_i|H|\psi_j\rangle$**
- **Partition the problem in a convenient manner**
  - — **particles in orbits, e.g., $0d_{5/2}(4)$, $1s_{1/2}(2)$, $0d_{3/2}(2)$.**
- **Assume GOE for each partition**
- **Evaluate partial level densities $\rho_\alpha(E)$, $\rho(E)=\Sigma_\alpha \rho_\alpha(E)$**

$$\rho_\alpha(E) = tr\left[P_\alpha \delta\left(E - \hat{H}\right)\right] \approx -\frac{1}{\pi}\left\langle \mathrm{Im}\, tr\left[P_\alpha \frac{1}{E - \hat{H} + i\eta}\right]_{\eta\to 0}\right\rangle$$

Statistical Method #1: Pluhar & Weidenmüller - 2

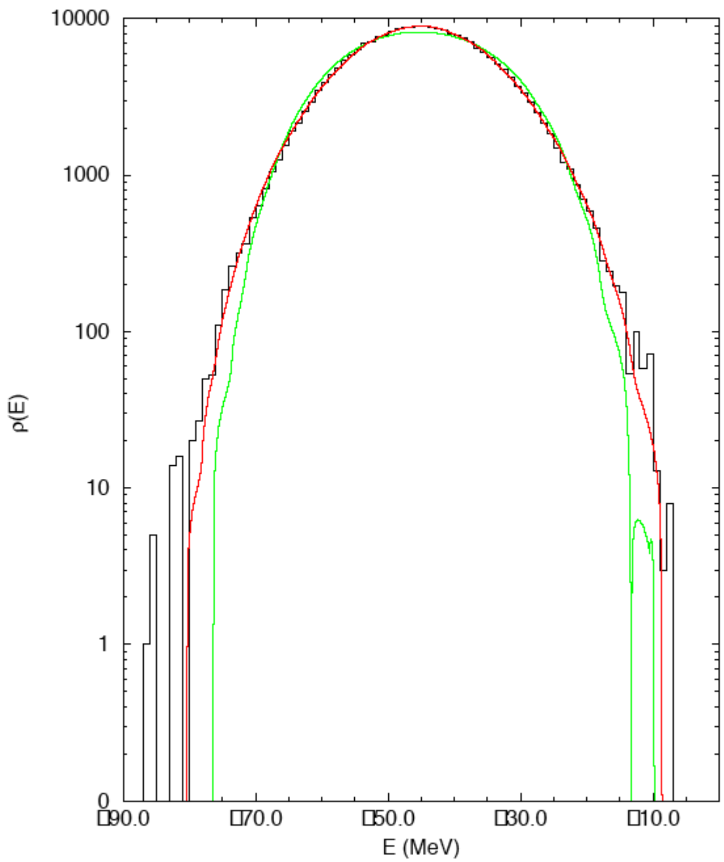
$$\rho(E) = \sum_{\alpha} \rho_{\alpha}(E)$$

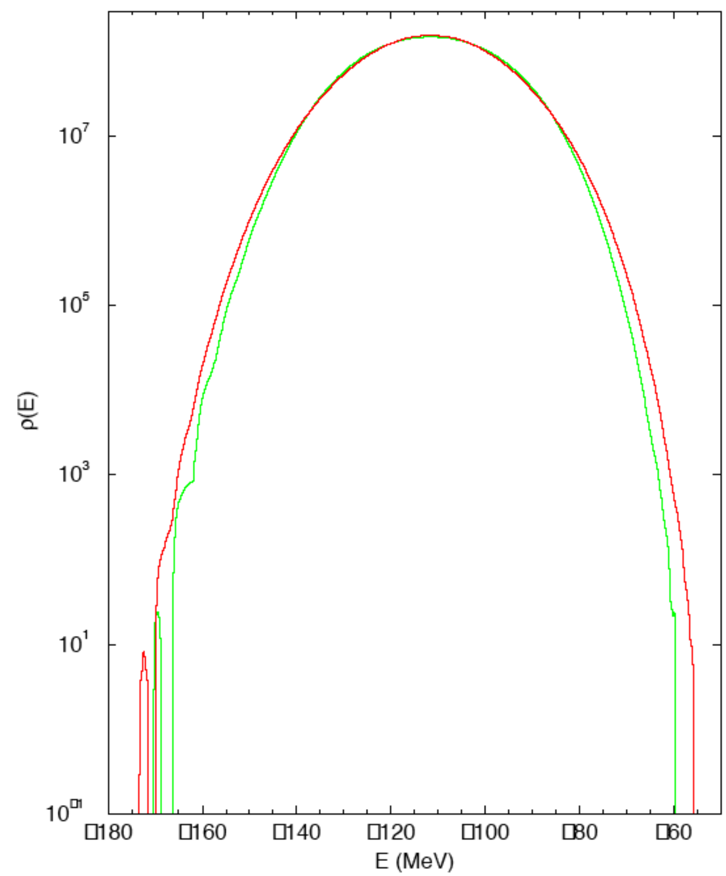
$$\rho_{\alpha}(E) = -\frac{1}{\pi} \mathrm{Im} \frac{1}{E - h_{\alpha} - \sigma_{\alpha}}, \quad \sigma_{\alpha} = \sum_{\beta} \frac{N_{\beta} \Gamma_{\alpha\beta}}{E - h_{\beta} - \sigma_{\beta}}$$



Statistical Method #1: Pluhar & Weidenmüller - 3

- ^{24}Mg and 54Fe state densities





Statistical Method with a binomial

- **J. Nabi, C.W. Johnson [LSU] and W.E. Ormand [LLNL]**
- **Level densities with two-body interactions are nearly Gaussian**
  - **Higher moments are somewhat different**
  - **Expand with Hermite polynomials**
    - **Not positive definite**
- **Try a binomial form – suggested by A. Zuker**

$$(1+\lambda)^N = \sum_{k=0}^{N} \lambda^k \binom{N}{k}$$

$$\lambda^k \binom{N}{k} = \text{ Number of levels at energy } E_x = \varepsilon k$$

$$\mu_1 = \frac{N\varepsilon\lambda}{1+\lambda}; \quad \mu_2 = \frac{N\varepsilon^2\lambda}{(1+\lambda)^2}; \quad \mu_3 = \frac{1-\lambda}{\sqrt{N\lambda}}\mu_2^{3/2}; \quad \mu_4 = \left(3 - \frac{4-\lambda}{N} + \frac{1}{N\lambda}\right)\mu_2^2$$

- **Fix μ_i with moments of the Hamiltonian**

$$\mu_1 = \overline{H} = \mathrm{Tr}(H); \qquad \mu_m = \mathrm{Tr}\left(\left(H - \overline{H}\right)^m\right)$$

Binomial

- **Improvement over Gaussian**
  - — **Includes μ_3**
  - — **Can correct Gaussian with orthogonal polynomials, i.e., Hermite**
    - – **Not guaranteed to be positive definite**
- **But fourth moment is determined by dimension *N***
  - — **Treat *N* as a parameter to fix μ_4 and scale ρ to get correct dimension – Fourth Moment Scaled (FMS)**
  - — **Sometimes it works really well**
  - — **Others it doesn't**

Improving the Binomial

- **Partition protons and neutrons in model space (144 for ^{24}Mg)**

$$\pi^2_{0d_{5/2}}\pi^1_{0d_{3/2}}\pi^1_{1s_{1/2}}\nu^2_{0d_{5/2}}\nu^2_{0d_{3/2}}\nu^0_{1s_{1/2}}$$

- **Compute moments of Hamiltonian:**

$$\mu_1 = \overline{H} = \mathrm{Tr}\left(P_a H\right); \qquad \mu_m = \mathrm{Tr}\left(P_a\left(H-\overline{H}\right)^m\right)$$

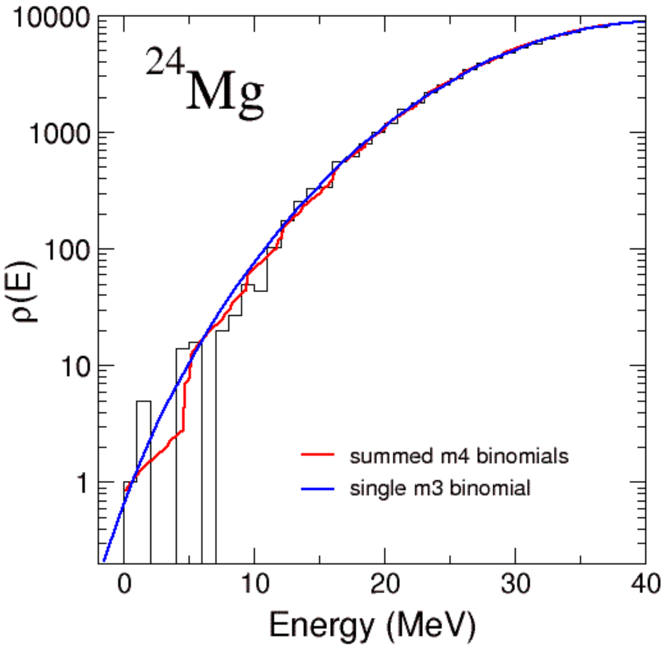
  — **Full influence on other partitions is accounted for, e.g.**

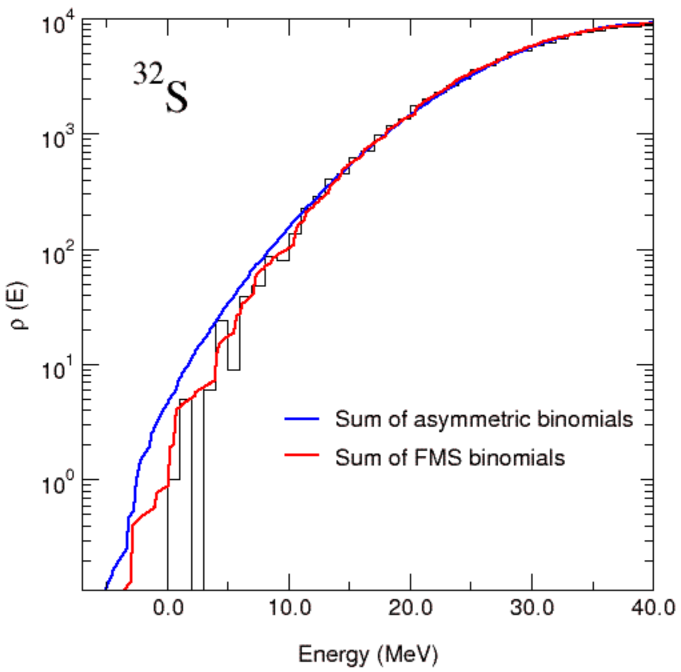
$$\mu_2^a = \sum_b \mathrm{Tr}\left(P_a\left(H-\overline{H}\right)P_b\left(H-\overline{H}\right)\right)$$

- **Assume partial level densities taken to have a binomial form and fix the moments**

$$\rho(E) = \sum_\alpha \rho_\alpha(E)$$

Application of a realistic model to compute $\rho(E)$





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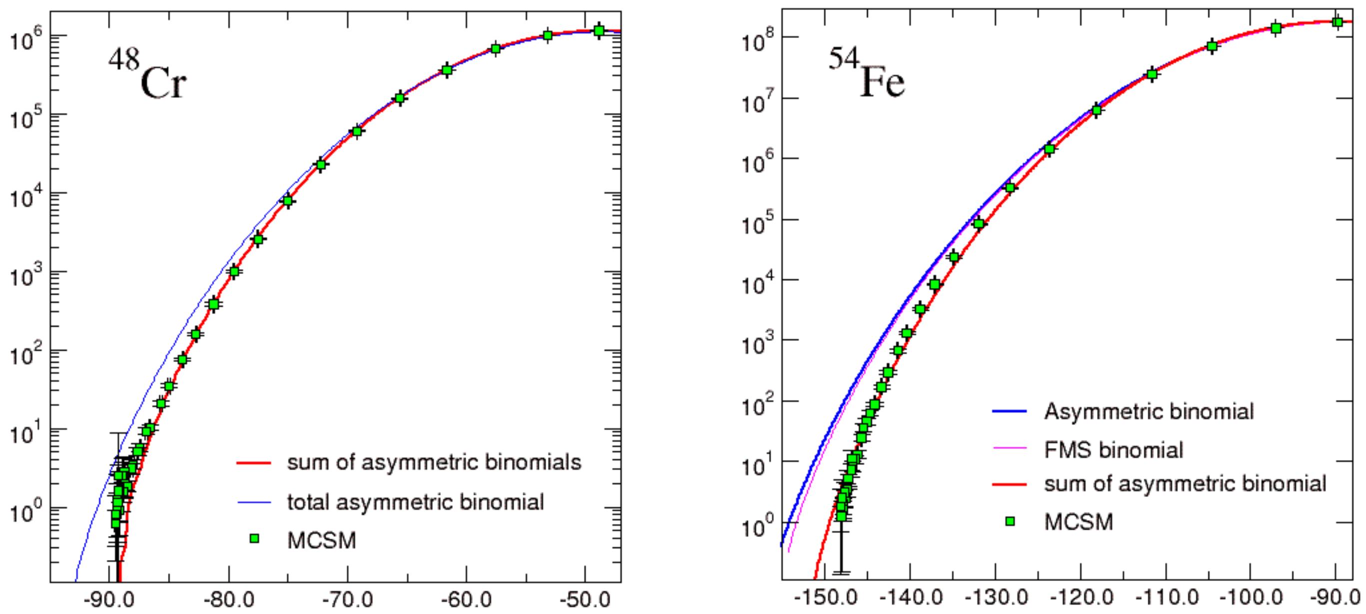
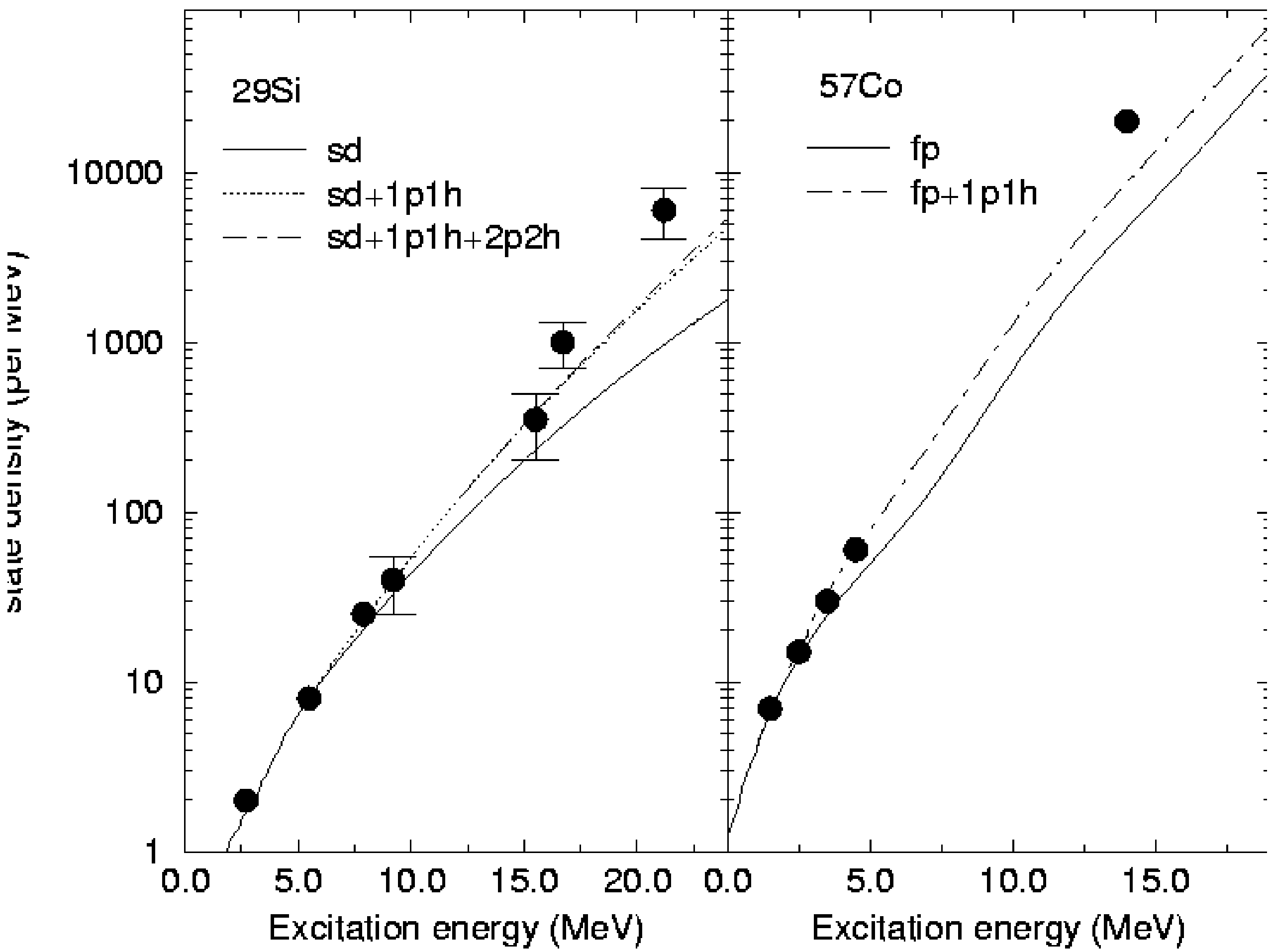
Application of a realistic model to compute $\rho(E)$



Application of a realistic model to compute *ρ(E)*



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The Good and the Bad

- **The Good**
  - — **Relatively fast**
    - – **Fourth moment can be expensive because of the number of partitions**
      - – **For ^{54}Fe about 24 hours (not yet optimized)**
      - – **But for MCSM over 700 hours**
      - – **Perhaps symmetric binomial may be good enough?**
  - — **Can use ANY interaction**
  - — **Parity distribution is trivial**
- **The Bad**
  - — **Limited by number of partitions**
  - — **Need two-body matrix elements for a “realistic” and meaningful Hamiltonian in the model space**
  - — **Can’t determine ground state energy with great accuracy ~ 500 keV**
    - – **Use MCSM?**
- **The unknown**
  - — **J projection and spin cut off parameter**